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2 Linear Models

2.1 General Linear Models

Any linear model can be written as

$y = X\beta + \epsilon$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

\uparrow

observed responses

$$= \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}$$

\uparrow

the elements of X are known (non-random) values

$$\begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

\uparrow

random errors are not observed

For the i -th case, the observed values are

$$(y_i \quad x_{i1} \quad x_{i2} \quad \cdots \quad x_{ik})$$

$\uparrow \qquad \qquad \uparrow$

response variable

explanatory variables that describe conditions under which the response was generated.

where ϵ specifying the distribution of the random error vector completes the specification of the distribution of y

Note:

$\epsilon = y - X\beta = y - E(y)$

Then,

$$E(\epsilon) = 0$$
$$V(\epsilon) = V(y) = \Sigma$$

Example 1. Regression Analysis:Yield of a chemical process

Yield (%)	Temperature ($^{\circ}F$)	Time (hr)
y	x_1	x_2
77	160	1
82	165	3
84	165	2
89	170	1
94	175	2

Simple linear regression model

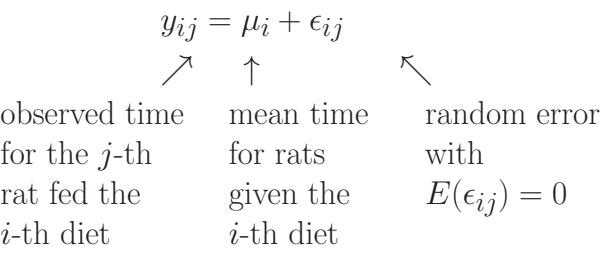
$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$$
$$i = 1, 2, 3, 4, 5$$

Matrix formulation:

Example 2.
Blood coagulation times (in seconds) for blood samples from six different rats. Each rat was fed one of three diets.

Diet 1	Diet 2	Diet 3
$y_{11} = 62$	$y_{21} = 71$	$y_{31} = 72$
$y_{12} = 60$		$y_{32} = 68$
		$y_{33} = 67$

A “means” model



You can express this model as

An “**effects**” model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

This can be expressed as

This is a linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} \quad \text{and} \quad V(\mathbf{y}) = \Sigma$$

You could add the assumptions

- independent errors
- homogeneous variance, i.e. $V(\epsilon_{ij}) = \sigma^2$

to obtain a linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} \quad \text{and} \quad V(\mathbf{y}) = \sigma^2 \mathbf{I}$$

Example 3. A 2×2 factorial experiment

- Experimental units: 8 plots with 5 trees per plot.
- Factor 1: Variety (A or B)
- Factor 2: Fungicide use (new or old)
- Response: Percentage of apples with spots

Percentage of apples with spots	Variety	Fungicide use
$y_{111} = 4.6$	A	new
$y_{112} = 7.4$	A	new
$y_{121} = 18.3$	A	old
$y_{122} = 15.7$	A	old
$y_{211} = 9.8$	B	new
$y_{212} = 14.2$	B	new
$y_{211} = 21.1$	B	old
$y_{222} = 18.9$	B	old

$$y_{ijk} = \mu + V_i + F_j + VF_{ij} + \epsilon_{ijk}$$

\uparrow

percent
with
spots

\uparrow

variety
effects
($i=1,2$)

\uparrow

fung.
use
($j=1,2$)

\uparrow

inter-
action
($k=1,2$)

\uparrow

random
error

Here we are using 9 parameters

$\beta^T = (\mu \ V_1 \ V_2 \ F_1 \ F_2 \ VF_{11} \ VF_{12} \ VF_{21} \ VF_{22})$
to represent the 4 response means,

$E(y_{ijk}) = \mu_{ij}, \quad i = 1, 2, \text{ and } j = 1, 2,$
corresponding to the 4 combinations of levels of
the two factors.
Write this model in the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

A “**means**” model

$$y_{ijk} = \mu_{ij} + \epsilon_{ijk}$$

where

$\mu_{ij} = E(y_{ijk})$ = mean percentage of apples with spots. This linear model can be written in the form $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, that is,

The “effects” linear model and the “means” linear model are equivalent in the sense that the space of possible mean vectors

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$

is the same for the two models.

- the model matrices differ
- the parameter vectors differ
- the columns of the model matrices span the same vector space

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$

$$= \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_k \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$$

$$= \beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2 + \cdots + \beta_k \mathbf{x}_k$$

2.2 Gauss-Markov Model

Definition 1.

The linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

is a **Gauss-Markov model** if

$$V(\mathbf{y}) = V(\boldsymbol{\epsilon}) = \sigma^2 I$$

for an unknown constant $\sigma^2 > 0$.

Notation: $\mathbf{y} \rightsquigarrow (\mathbf{X}\boldsymbol{\beta}, \sigma^2 I)$
 distributed as $E(\mathbf{y})$ $V(\mathbf{y})$

The distribution of \mathbf{y} is not completely specified.

2.3 Normal Theory Gauss-Markov Model

Definition 2.

A normal-theory Gauss-Markov model is a Gauss-Markov model in which \mathbf{y} (or $\boldsymbol{\epsilon}$) has a multivariate normal distribution.

$$\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 I)$$

\nearrow \uparrow \nwarrow \nwarrow
 distr. multivar. $E(\mathbf{y})$ $V(\mathbf{y})$
 as normal
 distr.

The additional assumption of a normal distribution is

- not needed for some estimation results
- useful in creating
 - confidence intervals
 - tests of hypotheses

2.4 Ordinary Least Squares Estimation

For the linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} \text{ and } V(\mathbf{y}) = \boldsymbol{\Sigma}$$

we have

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1k} \\ X_{21} & X_{22} & \cdots & X_{2k} \\ \vdots & \vdots & & \vdots \\ X_{n1} & X_{n2} & \cdots & X_{nk} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

and

$$\begin{aligned} y_i &= \beta_1 \mathbf{x}_{i1} + \beta_2 \mathbf{x}_{i2} + \cdots + \beta_k \mathbf{x}_{ik} + \epsilon_i \\ &= \mathbf{X}_i^T \boldsymbol{\beta} + \epsilon_i \end{aligned}$$

where $\mathbf{X}_i^T = (\mathbf{x}_{i1}, \mathbf{x}_{i2}, \dots, \mathbf{x}_{ik})$ is the i -th row of the model matrix \mathbf{X} .

Definition 3.

For a linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$, any vector \mathbf{b} that minimizes the sum of squared residuals

$$\begin{aligned} Q(\mathbf{b}) &= \sum_{i=1}^n (y_i - \mathbf{X}_i^T \mathbf{b})^2 \\ &= (\mathbf{y} - \mathbf{X}\mathbf{b})^T (\mathbf{y} - \mathbf{X}\mathbf{b}) \end{aligned}$$

is an ordinary least squares (OLS) estimator for $\boldsymbol{\beta}$.

For $j = 1, 2, \dots, k$, solve

$$0 = \frac{\partial Q(\mathbf{b})}{\partial b_j} = 2 \sum_{i=1}^n (y_i - \mathbf{X}_i^T \mathbf{b}) X_{ij}$$

Dividing by 2, we have

$$0 = \sum_{i=1}^n (y_i - \mathbf{X}_i^T \mathbf{b}) X_{ij} \quad j = 1, 2, \dots, k$$

These equations are expressed in matrix form as

$$\begin{aligned} \mathbf{0} &= \mathbf{X}^T (\mathbf{y} - \mathbf{X}\mathbf{b}) \\ &= \mathbf{X}^T \mathbf{y} - \mathbf{X}^T \mathbf{X}\mathbf{b} \end{aligned}$$

or

$$\mathbf{X}^T \mathbf{X}\mathbf{b} = \mathbf{X}^T \mathbf{y}$$

These are often called the “normal” equations.

If $\mathbf{X}_{n \times k}$ has full column rank, i.e., $\text{rank}(\mathbf{X}) = k$, then

- $\mathbf{X}^T \mathbf{X}$ is non-singular
- $(\mathbf{X}^T \mathbf{X})^{-1}$ exists and is unique

Consequently,

$$(\mathbf{X}^T \mathbf{X})^{-1}(\mathbf{X}^T \mathbf{X})\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1}\mathbf{X}^T \mathbf{y}$$

and

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1}\mathbf{X}^T \mathbf{y}$$

is the unique solution to the normal equations.

If $\text{rank}(\mathbf{X}) < k$, then

- there are infinitely many solutions to the normal equations
- if $(\mathbf{X}^T \mathbf{X})^{-}$ is a generalized inverse of $\mathbf{X}^T \mathbf{X}$, then

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y}$$

is a solution of the normal equations.

Example 4.

Suppose that we are interested in the coefficients $\boldsymbol{\beta}$ of a linear model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where \mathbf{Y} is $n \times 1$, \mathbf{X} is $n \times p$ and $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$. Furthermore, suppose that it is of interest to partition that model in the form $\mathbf{X} = [\mathbf{X}_1 \mathbf{X}_2 \mathbf{X}_3]$, for $n \times p_i$ matrices $\mathbf{X}_i, i = 1, 2, 3$. Finally, suppose that an investigator creates a partially orthogonal design, in which $\mathbf{X} = [\mathbf{X}_1 \mathbf{X}_2 \mathbf{X}_3]$ has the property that $\mathbf{X}_i^T \mathbf{X}_j = 0$ for $i \neq j$. Show that the least squares estimate of $\boldsymbol{\beta}$ takes the form $\hat{\boldsymbol{\beta}}$

$$= \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \end{bmatrix}, \text{ where}$$

- $\hat{\beta}_1 = (\mathbf{X}_1^T \mathbf{X}_1)^{-1} \mathbf{X}_1^T \mathbf{Y}$
- $\hat{\beta}_2 = (\mathbf{X}_2^T \mathbf{X}_2)^{-1} \mathbf{X}_2^T \mathbf{Y}$
- $\hat{\beta}_3 = (\mathbf{X}_3^T \mathbf{X}_3)^{-1} \mathbf{X}_3^T \mathbf{Y}$

2.5 Generalized Inverse

Definition 4.

For a given $m \times n$ matrix \mathbf{A} , any $n \times m$ matrix \mathbf{G} that satisfies

$$\mathbf{AGA} = \mathbf{A}$$

is a **generalized inverse** of \mathbf{A} .

Comments:

- (i) We will often use \mathbf{A}^- to denote a generalized inverse of \mathbf{A} .
- (ii) There may be infinitely many generalized inverses.
- (iii) If \mathbf{A} is an $m \times m$ nonsingular matrix, then $\mathbf{G} = \mathbf{A}^{-1}$ is the unique generalized inverse for \mathbf{A} .

Example 5.

$$\mathbf{A} = \begin{bmatrix} 16 & -6 & -10 \\ -6 & 21 & -15 \\ -10 & -15 & 25 \end{bmatrix} \text{ with } \text{rank}(\mathbf{A}) = 2.$$

Check that

$$\mathbf{G}_1 = \begin{bmatrix} \frac{1}{20} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{50} \end{bmatrix} \text{ and } \mathbf{G}_2 = \begin{bmatrix} \frac{21}{300} & \frac{6}{300} & 0 \\ \frac{6}{300} & \frac{16}{300} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

are generalized inverse of \mathbf{A} .**Example 6.**

A “means” model is as follow:

$$\begin{bmatrix} y_{11} \\ y_{12} \\ y_{21} \\ y_{31} \\ y_{32} \\ y_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \epsilon_{21} \\ \epsilon_{31} \\ \epsilon_{32} \\ \epsilon_{33} \end{bmatrix}$$

(i) Compute $\mathbf{X}^T \mathbf{X}$ and $\mathbf{X}^T \mathbf{y}$.

(ii) Obtain the OLS estimator.

Example 7.

“Effects” model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

$$i = 1, 2, 3; j = 1, 2, \dots, n_i$$

(i) Write out the $\mathbf{X}^T \mathbf{X}$ matrix for this models.

(ii) Check that $(\mathbf{X}^T \mathbf{X})^- = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{n_1} & 0 & 0 \\ 0 & 0 & \frac{1}{n_2} & 0 \\ 0 & 0 & 0 & \frac{1}{n_3} \end{bmatrix}$ is

a generalized inverses of $\mathbf{X}^T \mathbf{X}$ and compute the corresponding solution to the normal equations.

.

(iii) Another generalized inverse for $\mathbf{X}^T \mathbf{X}$ is

$$(\mathbf{X}^T \mathbf{X})^- = \begin{bmatrix} \begin{bmatrix} n_{\cdot} & n_1 & n_2 \end{bmatrix}^{-1} & 0 \\ n_1 & n_1 & 0 \\ n_2 & 0 & n_2 \\ 0 & 0 & 0 \end{bmatrix}$$

Compute the corresponding solution to the normal equations.

..

2.5.1 Evaluating Generalized Inverses

Step(1) Find any $r \times r$ nonsingular submatrix of \mathbf{A} where $r = \text{rank}(\mathbf{A})$. Call this matrix \mathbf{W} .

Step(2) Invert and transpose \mathbf{W} , ie., compute $(\mathbf{W}^{-1})^T$.

Step(3) Replace each element of \mathbf{W} in \mathbf{A} with the corresponding element of $(\mathbf{W}^{-1})^T$

Step(4) Replace all other elements in \mathbf{A} with zeros.

Step(5) Transpose the resulting matrix to obtain \mathbf{G} , a generalized inverse for \mathbf{A} .

Example 8.

$$\mathbf{A} = \begin{bmatrix} 4 & 1 & 2 & 0 \\ 1 & \textcircled{1} & \textcircled{5} & 15 \\ 3 & \textcircled{1} & \textcircled{3} & 5 \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} 1 & 5 \\ 1 & 3 \end{bmatrix}$$

You are given that $\text{rank}(\mathbf{A}) = 2$, find $\mathbf{G} = \mathbf{A}^-$.

Example 9.

$$\mathbf{A} = \begin{bmatrix} \textcircled{4} & 1 & 2 & \textcircled{0} \\ 1 & 1 & 5 & 15 \\ \textcircled{3} & 1 & 3 & \textcircled{5} \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} 4 & 0 \\ 3 & 5 \end{bmatrix}$$

You are given that $\text{rank}(\mathbf{A}) = 2$, find $\mathbf{G} = \mathbf{A}^-$.

.

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Example 12.

Show that $\mu + \alpha_3$ is estimable.

Example 13.

Show that $\alpha_1 - \alpha_2$ is estimable.

Example 14.

Show that $2\mu + 3\alpha_1 - \alpha_2$ is estimable.

2.7.2 Quantities that are not estimable

Quantities that are **not** estimable include

$$\mu, \alpha_1, \alpha_2, \alpha_3, 3\alpha_1, 2\alpha_2$$

To show that a linear function of parameters

$$c_0\mu + c_1\alpha_1 + c_2\alpha_2 + c_3\alpha_3$$

is not estimable, one must show that there is no non-random vector

$$\mathbf{a}^T = (a_0, a_1, a_2, a_3)$$

For which

$$E(\mathbf{a}^T \mathbf{y}) = c_0\mu + c_1\alpha_1 + c_2\alpha_2 + c_3\alpha_3$$

Example 15.

Show that α_1 is not estimable.

Result 5.

For a model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(y) = \boldsymbol{\Sigma}$:

- (i) The expectation of any observation is estimable.
- (ii) A linear combination of estimable functions is estimable.
- (iii) Each element of $\boldsymbol{\beta}$ is estimable if and only if $\text{rank}(\mathbf{X}) = k = \text{number of columns}$.
- (iv) Every $\mathbf{c}^T \boldsymbol{\beta}$ is estimable if and only if $\text{rank}(\mathbf{X}) = k = \text{number of columns in } \mathbf{X}$.

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Result 6. For a linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \Sigma$, each of the following is true if and only if $\mathbf{c}^T\boldsymbol{\beta}$ is **estimable**.

- (i) $\mathbf{c}^T = \mathbf{a}^T\mathbf{X}$ for some \mathbf{a} i.e., \mathbf{c} is in the space spanned by the rows of \mathbf{X} .
- (ii) $\mathbf{c}^T\mathbf{a} = 0$ for every \mathbf{a} for which $\mathbf{X}\mathbf{a} = \mathbf{0}$.
- (iii) $\mathbf{c}^T\mathbf{b}$ is the same for any solution to the normal equations $(\mathbf{X}^T\mathbf{X})\mathbf{b} = \mathbf{X}^T\mathbf{y}$, i.e., there is a **unique** least squares estimator for $\mathbf{c}^T\boldsymbol{\beta}$.

.

Example 16.

Use Result 6 (ii) to show that μ is not estimable.

Part (ii) of Result 6 sometimes provides a convenient way to identify all possible estimable functions of $\boldsymbol{\beta}$.

In Blood Coagulation Times example,

$$\mathbf{X}\mathbf{d} = \mathbf{0}$$

if and only if

$$\mathbf{d} = w \begin{bmatrix} 1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

for some scalar w .

Then,

$$\mathbf{c}^T \boldsymbol{\beta}$$

is estimable if and only if

$$0 = \mathbf{c}^T \mathbf{d} = w(c_1 - c_2 - c_3 - c_4) = 0$$

$$\iff c_1 = c_2 + c_3 + c_4.$$

Then,

$$(c_2 + c_3 + c_4)\mu + c_2\alpha_1 + c_3\alpha_2 + c_4\alpha_3$$

is estimable for any $(c_2 \ c_3 \ c_4)$ and these are the only estimable functions of $\mu, \alpha_1, \alpha_2, \alpha_3$.

For example, some estimable functions are

$$\mu + \frac{1}{3}(\alpha_1 + \alpha_2 + \alpha_3) \quad (c_2 = c_3 = c_4 = \frac{1}{3})$$

and

$$\mu + \alpha_2 \quad (c_2 = 1 \ c_3 = c_4 = 0)$$

but

$$\mu + 2\alpha_2$$

is not estimable

Example 17.

Let

$$\mathbf{y} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix}$$

Show that every linear parametric function $c_1\beta_1 + c_2\beta_2$ is estimable.

Example 18. Consider the model

$$y_{ijk} = \mu + \alpha_i + \beta_j + \epsilon_{ijk}, i = 1, 2; j = 1, 2; k = 1.$$

Describe the set of estimable functions of μ , α 's and β 's.

Definition 7.

For a linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \Sigma$, where \mathbf{X} is an $n \times k$ matrix, $C_{r \times k}\boldsymbol{\beta}_{k \times 1}$ is said to be **estimable** if all of its elements

$$C\boldsymbol{\beta} = \begin{bmatrix} \mathbf{c}_1^T \\ \mathbf{c}_2^T \\ \vdots \\ \mathbf{c}_r^T \end{bmatrix} \boldsymbol{\beta} = \begin{bmatrix} \mathbf{c}_1^T \boldsymbol{\beta} \\ \mathbf{c}_2^T \boldsymbol{\beta} \\ \vdots \\ \mathbf{c}_r^T \boldsymbol{\beta} \end{bmatrix}$$

are estimable.

Result 8. Gauss-Markov Theorem

For the Gauss-Markov model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} \text{ and } V(\mathbf{y}) = \sigma^2I$$

the OLS estimator of an estimable function $\mathbf{c}^T\boldsymbol{\beta}$ is the **unique** best linear unbiased estimator (blue) of $\mathbf{c}^T\boldsymbol{\beta}$.

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Example 19.
The response time in milliseconds was determined for three different types of circuits that could be used in an automatic valve shutoff mechanism. The results are shown in the following table.

Circuit Type	Response Time				
1	9	12	10	8	15
2	20	21	23	17	30
3	6	5	8	16	7

Consider the model

$$y_{ij} = \mu + \tau_i + \epsilon_{ij}; i = 1, 2, 3; j = 1, 2, 3, 4, 5$$

where μ is the overall mean, τ_i is the circuit type content effects and $\epsilon_{ij} \sim N(0, \sigma^2)$ is the random error. Compute the BLUE of $\tau_1 - 2\tau_2 + \tau_3$

estimator $\hat{\Sigma}$ for Σ .

- use method of moments or maximum likelihood estimation to obtain $\hat{\Sigma}$
- the resulting estimator
 - * is not a linear estimator
 - * is consistent but not necessarily unbiased
 - * does not provide a blue for estimable functions
 - * may have larger mean squared error than the OLS estimator

To create confidence intervals or test hypotheses about estimable functions for a linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta} \text{ and } V(\mathbf{y}) = \Sigma$$

we must

- (i) specify a probability distribution for \mathbf{y} so we can derive a distribution for

$$\mathbf{c}^T \mathbf{b} = \mathbf{c}^T (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-1} \mathbf{X}^T \Sigma^{-1} \mathbf{y}$$

- (ii) estimate σ^2 when

$$V(\mathbf{y}) = \sigma^2 I \text{ or } V(\mathbf{y}) = \sigma^2 V$$

for some known V .

- (iii) Estimate Σ when

$$V(\mathbf{y}) = \Sigma$$

Example 20.

Suppose that y_{11} and y_{12} are independent $N(\mu_1, \eta)$ variables independent of y_{21} and y_{22} that are independent $N(\mu_2, 4\eta)$ variables. (The η and 4η are variances.) What is the BLUE of $\mu_1 - \mu_2$? Explain carefully.

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Example 21.

Suppose $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$, where for $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \dots, \epsilon_n)'$, $E(\boldsymbol{\epsilon}) = \mathbf{0}$. A particular experiment produces $n = 5$ data points as per table below:

x	1	2	3	4	5
y	9	6	4	3	2

Suppose that $V(\epsilon) = \sigma^2 diag(1, 4, 9, 25)$.

- (i) Give a matrix \mathbf{T} such that $\mathbf{T}\mathbf{y}$ follows a Gauss- Markov model.

(ii) What is the model matrix for $\mathbf{T}\mathbf{y}$?

(iii) Evaluate an appropriate point estimate of β under these model assumptions.

The models are “equivalent”: the space spanned by the columns of \mathbf{W} is the same as the space spanned by columns of X .

You can find matrices F and \mathbf{G} such that

$$\mathbf{W} = X \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = XF$$

and

$$X = \mathbf{W} \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix} = \mathbf{W}\mathbf{G}$$

Then,

$$(i) \text{rank}(X) = \text{rank}(\mathbf{W})$$

(ii) Estimated mean responses are the same:

$$\begin{aligned} \hat{\mathbf{y}} &= X(X^T X)^{-1} X^T \mathbf{y} \\ &= \mathbf{W}(\mathbf{W}^T \mathbf{W})^{-1} \mathbf{W}^T \mathbf{y} \end{aligned}$$

or

$$\hat{\mathbf{y}} = P_X \mathbf{y} = P_{\mathbf{W}} \mathbf{y}$$

(iii) Residual vectors are the same

$$\begin{aligned} \mathbf{e} &= \mathbf{y} - \hat{\mathbf{y}} = (I - P_X) \mathbf{y} \\ &= (I - P_{\mathbf{W}}) \mathbf{y} \end{aligned}$$

Example 23. Regression model for the yield of a chemical process

$$y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \epsilon_i$$

\uparrow \uparrow \uparrow
 yield temperature time

An “equivalent” model is

$$y_i = \alpha_0 + \beta_1(X_{1i} - \bar{X}_{1.}) + \beta_2(X_{2i} - \bar{X}_{2.}) + \epsilon_i$$

For the first model:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{21} \\ 1 & X_{12} & X_{22} \\ 1 & X_{13} & X_{23} \\ 1 & X_{14} & X_{24} \\ 1 & X_{15} & X_{25} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

For the second model:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} \begin{bmatrix} 1 & X_{11} - \bar{X}_1 & X_{21} - \bar{X}_2 \\ 1 & X_{12} - \bar{X}_1 & X_{22} - \bar{X}_2 \\ 1 & X_{13} - \bar{X}_1 & X_{23} - \bar{X}_2 \\ 1 & X_{14} - \bar{X}_1 & X_{24} - \bar{X}_2 \\ 1 & X_{15} - \bar{X}_1 & X_{25} - \bar{X}_2 \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix} = \mathbf{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

The space spanned by the columns of X is the same as the space spanned by the columns of \mathbf{W} . Find matrices \mathbf{G} and F such that $X = \mathbf{W}\mathbf{G}$ and $\mathbf{W} = XF$.

Definition 9.

Consider two linear models:

1. $E(\mathbf{y}) = X\boldsymbol{\beta}$ and $V(\mathbf{y}) = \boldsymbol{\Sigma}$ and,

2. $E(\mathbf{y}) = \mathbf{W}\boldsymbol{\gamma}$ and $V(\mathbf{y}) = \boldsymbol{\Sigma}$

where X is an $n \times k$ model matrix and \mathbf{W} is an $n \times q$ model matrix.

We say that one model is a **reparameterization** of the other if there is a $k \times q$ matrix F and a $q \times k$ matrix \mathbf{G} such that

$$\mathbf{W} = XF \text{ and } X = \mathbf{W}\mathbf{G}.$$

The previous examples illustrate that if one model is a reparameterization of the other, then

(i) $\text{rank}(X) = \text{rank}(\mathbf{W})$

(ii) Least squares estimates of the response means are the same, i.e., $\hat{\mathbf{y}} = P_X\mathbf{y} = P_{\mathbf{W}}\mathbf{y}$

(iii) Residuals are the same, i.e.,

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = (I - P_X)\mathbf{y} = (I - P_{\mathbf{W}})\mathbf{y}$$

(iv) An unbiased estimator for σ^2 is provided by

$$MSE = SSE/(n - \text{rank}(X))$$

where,

$$\begin{aligned} SSE &= \mathbf{e}^T \mathbf{e} = \mathbf{y}^T (I - P_X) \mathbf{y} \\ &= \mathbf{y}^T (I - P_{\mathbf{W}}) \mathbf{y} \end{aligned}$$

Reasons for reparameterizing models:

(i) Reduce the number of parameters

- Obtain a full rank model
- Avoid use of generalized inverses

(ii) Make computations easier

- In the previous examples, $\mathbf{W}^T \mathbf{W}$ is a diagonal matrix and $(\mathbf{W}^T \mathbf{W})^{-1}$ is easy to compute

(iii) More meaningful interpretation of parameters.

Result 10.

Suppose two linear models,

$$(1) \quad E(\mathbf{y}) = X\boldsymbol{\beta} \quad V(\mathbf{y}) = \boldsymbol{\Sigma}$$

and

$$(2) \quad E(\mathbf{y}) = \mathbf{W}\boldsymbol{\gamma} \quad V(\mathbf{y}) = \boldsymbol{\Sigma}$$

are reparameterizations of each other, and let F be a matrix such that $\mathbf{W} = XF$. Then

(i) If $\mathbf{C}^T\boldsymbol{\beta}$ is estimable for the first model, then $\boldsymbol{\beta} = F\boldsymbol{\gamma}$ and $\mathbf{C}^TF\boldsymbol{\gamma}$ is estimable under Model 2.

(ii) Let $\hat{\boldsymbol{\beta}} = (X^TX)^-X^T\mathbf{y}$ and $\hat{\boldsymbol{\gamma}} = (\mathbf{W}^T\mathbf{W})^-\mathbf{W}^T\mathbf{y}$. If $\mathbf{C}^T\boldsymbol{\beta}$ is estimable, then

$$\mathbf{C}^T\hat{\boldsymbol{\beta}} = \mathbf{C}^TF\hat{\boldsymbol{\gamma}}$$

(iii) if $H_0 : \mathbf{C}^T\boldsymbol{\beta} = \mathbf{d}$ is testable under one model, then $H_0 : \mathbf{C}^TF\boldsymbol{\gamma} = \mathbf{d}$ is testable under the other.

Example 24.

Consider a problem of quadratic regression in one variable, X . In particular, suppose that $n = 5$ values of a response y are related to values $x = 0, 1, 2, 3, 4$ by a linear model $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ for

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix}, \quad X = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \quad \text{and} \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

Define

$$\mathbf{W} = \begin{bmatrix} 1 & -2 & 2 \\ 1 & -1 & -1 \\ 1 & 0 & -2 \\ 1 & 1 & -1 \\ 1 & 2 & 2 \end{bmatrix}$$

- (a) Formulate what is meant by the statement that $\mathbf{y} = \mathbf{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$ is a reparameterization of $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$.

- (b) Show that $\mathbf{y} = \mathbf{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$ is reparameterization of $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where $\boldsymbol{\gamma}^T = [\gamma_1, \gamma_2, \gamma_3]$.

- (c) Notice that $\mathbf{W}^T\mathbf{W}$ is diagonal. Suppose that $\mathbf{y}^T = (-2, 0, 4, 2, 2)$. Find the OLS estimate of $\boldsymbol{\gamma}$ in the model $\mathbf{y} = \mathbf{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$ and then OLS estimate of $\boldsymbol{\beta}$ in the original model. (Find numerical values.)

2.11 Restrictions (side conditions)

- Give meaning to individual parameters
- Make individual parameters estimable
- Create a full rank model matrix
- Avoid the use of generalized inverses
- Restrictions must involve "non-estimable" quantities for the unrestricted "effects" model.

Example 25. An effects model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

This model can be expressed as

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

Impose the restriction

$$\alpha_3 = 0$$

Then, $E(y_{1j}) =$

$$E(y_{2j}) =$$

$$E(y_{3j}) =$$

and

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

Write this model as $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where

$$X = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \end{bmatrix} \text{ and } \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix}$$

Then, $X^T X =$

and

$X^T \mathbf{y} =$

and the unique OLS estimator for $\boldsymbol{\beta} = (\mu \ \alpha_1 \ \alpha_2)^T$ is

Example 26.
Consider the model $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ with the restriction $\alpha_1 + \alpha_2 + \alpha_3 = 0$. Then, $\alpha_3 = -\alpha_1 - \alpha_2$ and

$E(y_{1j}) =$
 $E(y_{2j}) =$
 $E(y_{3j}) =$ and

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ \vdots & \vdots & \vdots \\ 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

This model is $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$

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The unique OLS estimator for $\boldsymbol{\beta} = (\mu \ \alpha_1 \ \alpha_2)^T$ is

Example 27.
Consider the model $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ with the restriction $\alpha_1 = 0$. Then,

$E(y_{1j}) =$
 $E(y_{2j}) =$
 $E(y_{3j})$
and

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_2 \\ \alpha_3 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

This model is $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$, with

$$X = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \end{bmatrix} \text{ and } \boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_2 \\ \alpha_3 \end{bmatrix}$$

The unique OLS estimator for $\boldsymbol{\beta} = (\mu \ \alpha_1 \ \alpha_2)^T$ is

The restrictions (i.e. the choice of one particular solution to the normal equations) have no effect on the OLS estimates of estimable quantities.

The estimated treatment means are:

$$E(\hat{y}_{1j}) = \hat{\mu} = \bar{y}_1.$$

$$E(\hat{y}_{2j}) = \hat{\mu} + \hat{\alpha}_2 = \bar{y}_2.$$

$$E(\hat{y}_{3j}) = \hat{\mu} + \hat{\alpha}_3 = \bar{y}_3.$$